

VSTAR Modelling of the Infrared Spectrum of Uranus

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Summary: We modelled the H-band spectrum obtained with the Infrared Imaging Spectrograph (IRIS2) at the Anglo-Australian Telescope in order to infer the cloud structure and composition of the atmosphere of the planet between 0.1 and 11 bar. Such modelling can be used to derive the D/H ratio in the atmosphere of Uranus, which is an important diagnostic of the conditions in early history of the planetary formation. We describe here our modelling technique based on the Versatile Software for Transfer of Atmospheric Radiation (VSTAR) [1]. Since the infrared spectrum of Uranus is dominated by absorption from methane, the accuracy of the models is limited largely by the quality of the low temperature, CH₄ line databases used. Our modelling includes the latest laboratory line data for methane described in Bailey 2011 [2]. The parameters of this model will be applied in the future to model our observations of GNIRS high resolution spectra of Uranus and derive the D/H ratio in the 1.58 μ m window based on absorption in the CH₃D band in this region.

Keywords: Uranus, modelling, spectroscopy, atmospheres, cloud structure

Introduction

The gas giant Uranus, with its 98° spin-axis inclination [3] has the largest variation in the amount of solar radiation received of any planet as one pole pointing nearly to the sun at a point in the orbit, becomes the pole pointing nearly away from the sun at the opposite point in the orbit. However the lack of an internal heat source combined with the long radiative time constant is the most likely reason that its atmosphere appears rather devoid of the band-like features characteristic for Jupiter or Saturn [4]. The aquamarine colour of the planet is attributed to methane absorption in visible light.

After the flyby of Voyager 2 in 1986 [5], detailed imaging and spectroscopy measurements confirmed that molecular hydrogen and helium (0.152 molar fraction) are the main constituents of the planet's atmosphere. The next most abundant component is methane with a mixing ratio of about 2%, followed by traces of ammonia, water and hydrogen sulphide. The radio occultation measurements suggested the existence of a thick methane cloud layer in the troposphere at 1.2 bar. Methane freezes out in the higher levels of the atmosphere and its mixing ratio drops below 5×10^{-3} at pressures lower than 500mb. A haze of complex hydrocarbons in the stratosphere (at pressures below 20 mbar) was suggested by Spitzer Telescope 20 μ m observations [6] and occultation measurements with the UV spectrometer on Voyager 2 [7]. Clouds of water, ammonia and hydrogen sulphide are expected to form in the lower troposphere at pressures above 3 bar. The top of the highest deck of ammonia or hydrogen sulphide clouds was derived based on the optical spectrum in Irwin 2010 [8].

Discrete clouds were first imaged by Voyager 2 [9] and later by Keck and Hubble Space telescopes [10] in the near-infrared range. The highest clouds at 200 mbar were visible in

the K-band, while imaging and J and H band spectroscopy showed cloud features at 2 to 5 bar in so-called "methane windows", where the atmosphere is transparent to almost 10 bar. Observations of discrete clouds allow measurement of the atmospheric circulation and zonal wind speeds at different heights. Seasonal and longitudinal variations in albedo due to inhomogeneity of aerosols over the disk of Uranus have been detected and discussed in Kostogryz 2007 [11].

Karkoshka and Tomasko 2009 [12] analysed a number of spatially resolved spectra of Uranus obtained with the STIS Hubble spectrograph in a range between 0.3 and 1 μm and found evidence of changes in the mixing ratio of methane at different latitudes, with higher mixing ratios at lower latitudes. This is consistent with the suggestion of a meridional flow with descending gas at high latitudes [13]. Irwin 2010 [14] used the latest methane line data (available from Campargue 2012 [15]) to model the near-infrared spectra from Gemini North NIFS data to better constrain methane abundance, the height of the top of the main cloud and the $\text{CH}_3\text{D}/\text{CH}_4$ ratio. Their results suggest that the thickness and the height of the main cloud varies as a function of latitude. The cloud deck appears highest at around 45° North and South of equator and it thickens towards the equator.

In this paper we describe our collection and reduction methods in the "Observations" section. We then describe the Fortran code, VSTAR, used to model a comparison spectrum and describe the considerations that went into setting the model up such as the methane mixing ratio and why it is important, other sources of absorption, scattering sources and the structure of the clouds. We then discuss the deuterium abundance and its importance before concluding with comments on the abilities of VSTAR, the importance of deuterium measurement and the possibility of better confining the deuterium amounts with new, higher resolution spectra.

Observations

On the 31st of July 2010 we acquired long-slit (7.7 arcmin) spectra of Uranus with the InfraRed Imaging Spectrograph (IRIS2) at the Anglo-Australian Telescope. The observations were taken with a resolving power of $R \sim 2400$ over the J, H and K bands, which covers the wavelength region between 1.09 to $2.4 \mu\text{m}$. For the H band, of which this paper is primarily concerned the signal to noise ratio was sufficiently high that it did not affect the quality of the fits. The 1 arcsec wide slit was oriented north-south on the sky, but the axis of Uranus is at a position angle of 254° (measured E from N), so our slit crosses mostly equatorial regions of the planet. The width of the slit is equivalent to 2.2 pixels on the detector. Our observing strategy was to take a sequence of four exposures (A, B, B, A) where A and B denote frames with the planet offset to two different positions on the slit. Observations were taken in 16 cycles of 1.5s x 41 exposures giving us a total exposure time of 960 seconds.

The spectra were extracted using the standard data reduction package FIGARO [16]. We carried out flat-field correction of the 2D spectra in order to remove the non-uniform response of the detector. Wavelength calibration was achieved with a xenon line source. Sky subtraction was performed by subtracting two corresponding frames with offset spectra (A and B) from each other. We also corrected for spectral curvature by resampling the frames using the spectra of standard stars taken for each band. In addition we removed bad pixels due to cosmic rays and known imperfections of the detector by interpolating between their neighbours. Our sun-like, G-type, standard stars used for flux calibration and removal of telluric absorption

were observed at close angular proximity to the planet. The absolute radiance factor, I/F , which compares the planet's reflected intensity to its received flux over given wavelengths (as discussed in [17]), is derived by dividing the extracted spectrum of Uranus by the spectrum of the standard star.

Figure 1 shows the resulting spectrum at the J, H and K bands.

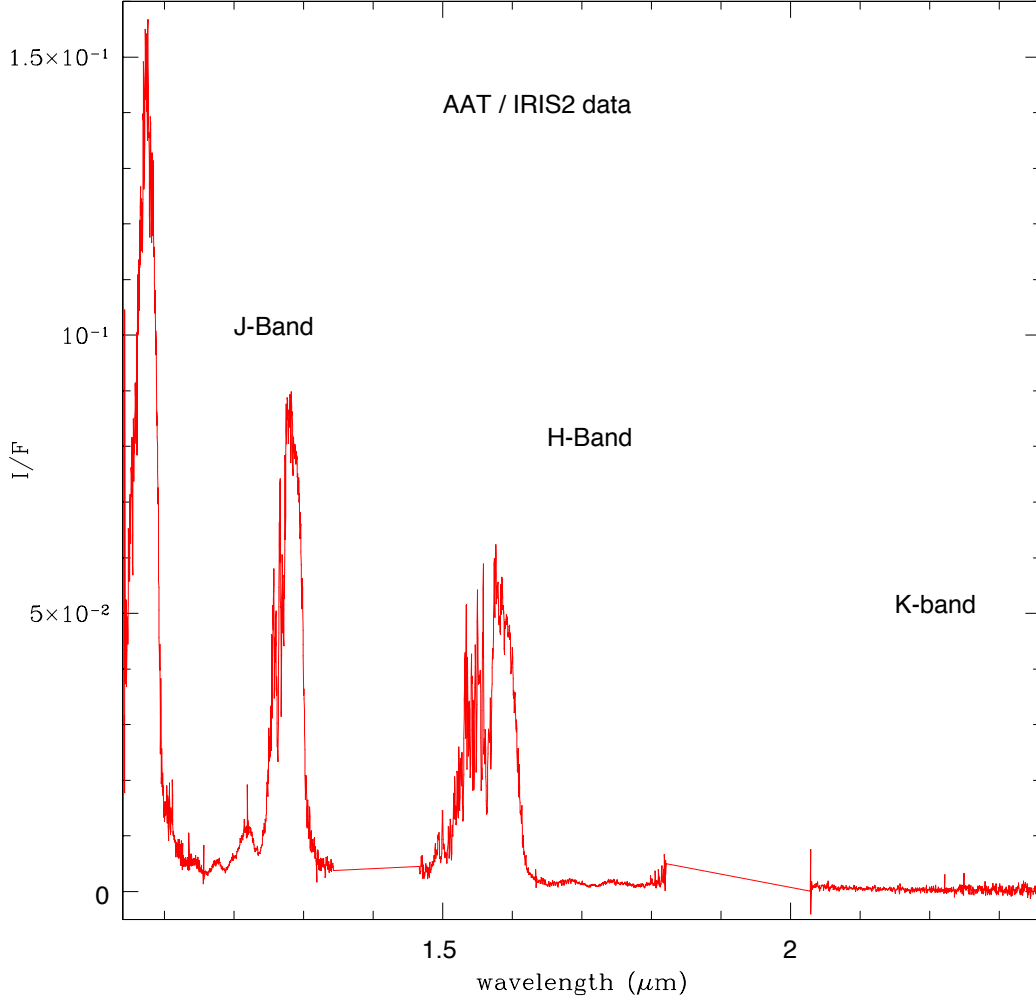


Fig. 1: The spectrum of Uranus in the near-infrared region observed with the IRIS2 instrument at the AAT on 31/07/10 with a resolution of 2400

VSTAR model of the H-band spectrum

To obtain the best fit for our observed spectrum we used the Versatile Software for Transfer of Atmospheric Radiation (VSTAR), which is a modular, line-by-line atmospheric radiative transfer package described in Bailey and Kedziora-Chudczer 2012 [1]. It has been successfully applied to planets of the Solar system: Earth [18], Venus [19] [20], Jupiter [17]; planetary moons such as Titan [2] [21] [22] and brown dwarfs [1]. The newly extended version of the software also allows modelling the spectra of transiting extrasolar planets and it can solve for fully polarised radiation transfer.

VSTAR is a Fortran code that calculates the radiative transfer of light in an atmosphere that can have a multilayer structure, where each layer has a defined chemical composition and scattering particle properties. The VSTAR modelling code is organised as a Fortran subroutine library from which a specific model is built by writing a simple program that calls appropriate routines. The MOD package defines a two dimensional grid of parameters for each atmospheric layer as a function of wavelength or a wave number. The parameters of the atmosphere such as pressure and temperature for every layer are either known from direct measurements or can be solved for in a similar way as described in Hubeny 1995 [23]. The LIN package is used to read spectral lines from line databases [2] and the RAY package derives optical depth due to Rayleigh scattering due to molecules. The PART module is used next to derive scattering properties of the aerosols and clouds. In this module, one specifies size distributions and refractive indices and optical depths for all particles present in different layers of the atmosphere and the scattering properties are calculated using Lorenz-Mie theory. The major component of the VSTAR package is the RT module, which contains a selection of radiative transfer solvers including DISORT adapted from Stanmes 1988 [24]. VSTAR was recently upgraded to allow a full four Stokes treatment of the polarized radiative transfer problem [25].

The spectrum of Uranus was modelled by dividing the atmosphere into 58 layers ranging from 0 to 136.5 km (or 11285 to 101 mbar) with the temperature-pressure (P-T) profile derived from radio occultations measured with Voyager 2 [26]. For this model we concentrated on the window surrounding $1.6\mu\text{m}$ because the K band for Uranus is low flux and databases for methane lines at the temperature of Uranus are not yet well developed for the J band.

Methane Mixing Ratio Profile and Absorption

The distribution of methane over these altitudes is not uniform and the profile of the methane mixing ratio almost certainly depends on the observed latitudes as well. The new, refined profile derived from Irwin et al. 2010 [27] (Figure 2) gave the best fit to our data. The CH_4 mixing ratio at the deepest levels of the atmosphere is 4%, which is higher than the 1.6% estimated from observations at polar latitudes at pressures higher than 1 bar [28]. This higher 4% mixing ratio is consistent with the P-T profile containing warmer lower layers of the atmosphere from occultation data [26], as can be seen in the left panel of Fig. 7 of Irwin 2010 [27]. Our slit, positioned at the centre of the planetary disk, covers a only a limited range of latitudes around the equator. Therefore the single methane profile from Irwin 2010 [27] is expected to account for the observed absorption features visible in our data.

Methane is the dominant absorbing species in the atmosphere of Uranus in the near infrared region. The CH_4 molecule has a complex absorption spectrum, which arises due to four vibrational modes interacting with each other, forming so-called polyads. Although there has been continuing progress in determination of the methane spectrum (see [21]), the high-order polyads, which form absorption lines in the near infrared ($1 - 2\mu\text{m}$) are not well understood. The HITRAN database at these wavelengths is largely based on empirical measurements at room temperature, but because their lower-state energies and quantum identifications are missing, it is difficult to model such lines for different temperatures.

A recent major breakthrough has been a set of deep laboratory measurements of methane lines at room temperature and cryogenic temperatures by the Grenoble group ([29], [30])

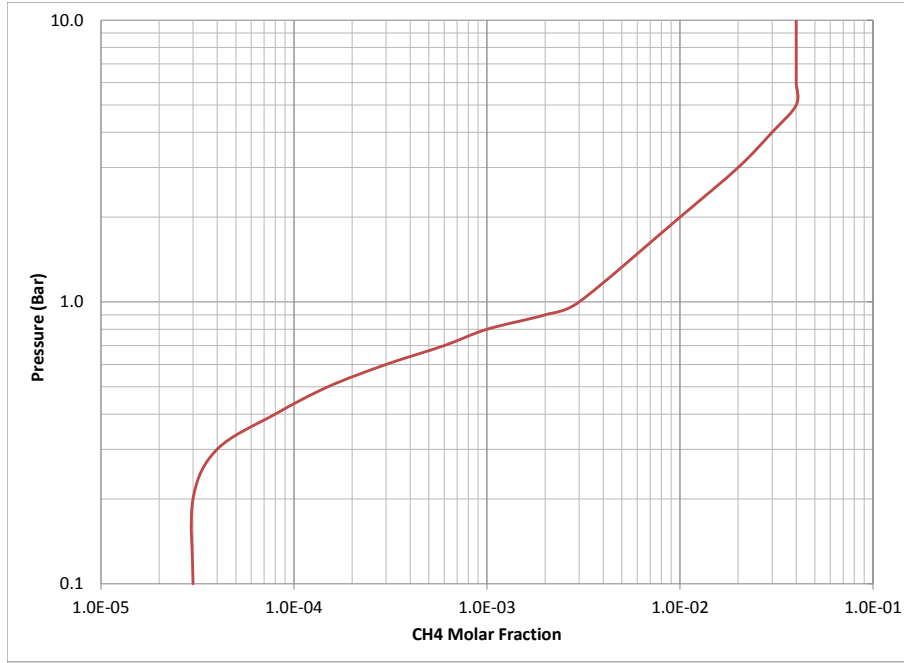


Fig. 2: Methane mixing ratio in the atmosphere of Uranus as a function of pressure.

which provide an excellent line list over the range $1.26 - 1.71 \mu\text{m}$. These line data have been shown to give good models for the spectra of Titan ([2], [21], [31]). We use a line list based on this new data, as well as other sources at longer wavelengths, as described in Bailey 2012 [21].

The shape of methane lines, especially in far wings of the strong lines has an effect on the shape of the absorption windows. In the H-band data we found that the best fit is achieved by using a Lorentzian profile with a cut-off at 100 cm^{-1} .

Other absorbers

The dominant component of the Uranian atmosphere is molecular hydrogen, which is not only the source of Rayleigh scattering, but also absorbs infrared radiation due to collisional interactions in a dense gas that induce electric dipoles that emit or absorb radiation at rotovibrational frequencies. This collision-induced absorption (CIA) gives rise to a spectrum of overlapping lines, which give the impression of a smooth absorption trough. Since the atmosphere of Uranus is about 15% helium, one has to consider also collisional interactions between H_2 and He molecules. We modelled both in our code based on coefficients derived in Borysow 1991 [32]. We note that CIA effects in H-band spectrum are likely to be rather small, because this is the region of low CIA absorption coefficients between two prominent bands: the fundamental and its first overtone. We have also assumed an equilibrium ortho/para H_2 -ratio in our model.

Scattering

Two sources of scattering are considered in our model. Rayleigh scattering cross sections due to molecules are calculated for an atmosphere composed of H_2 and He. Rayleigh scattering is most efficient at short wavelengths, so scattering in our infrared region will occur mainly due to clouds and aerosols that form hazes.

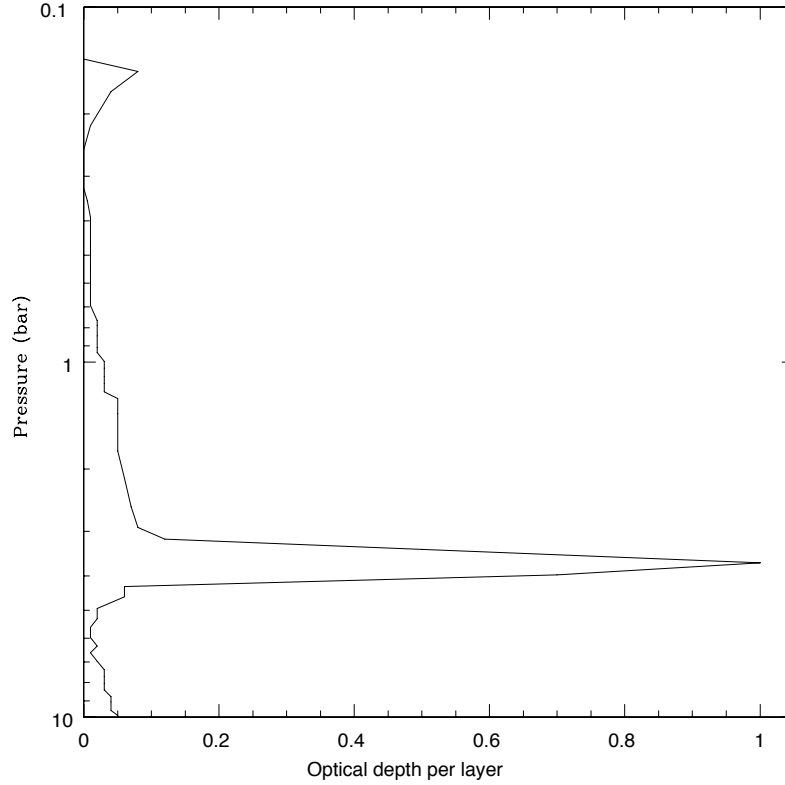


Fig. 3: Cloud opacity profile used for the model.

Lorenz-Mie theory is used to model scattering from the clouds. We assumed a power-law size distribution of particles with effective radius of $2\mu m$ and variance of $0.4\mu m$ with a constant complex refractive index of $n = 1.4 + 0i$ in the considered range of wavelengths. The phase function was modelled with a Henyey-Greenstein function. The cloud composition and particle size can change by height but we found no major effect on the spectrum by changing between 1.2 and $5\mu m$ sized particles.

The cloud optical depth profile presented in Figure 3 is consistent with the latest model from Irwin 2010 [27], where the 4% mixing ratio of methane was applied at pressures above 1 bar. This profile does not have a break in the lower cloud cover in the equatorial regions which was needed to provide good fit for modelling the data with lower mixing ratios of CH_4 used by Irwin et al. in the past [33]. We found that our model spectra required a low opacity haze present at the pressures from about 0.15 to 0.2 bar. Such a high altitude haze layer was previously necessary for the model fitting of Uranus used by other groups [12, 14]. For simplicity we assumed that the upper haze was made from particles of the same size as the lower cloud.

Fitting the structure and opacity of the cloud layers was done initially by manual analysis and manipulation of the opacity profile as a function of pressure. Irwin 2012 [14] notes the degeneracy between the choice of methane profile and the detailed structure of the cloud decks for latitudinally averaged spectra.

We compared models with cloud opacity profile adapted from Irwin 2012 [14] which included low altitude haze with the profile adopted from Karkoschka & Tomasko 2009 [12] for a single solid cloud and haze layer at pressures lower than 0.1 bar. Our spectrum was derived from the narrow range of latitudes around planetary equator, so we applied these cloud profiles to the mixing ratio profile that includes an enhanced methane abundance at deep levels of atmosphere [26]. We found that the cloud profile similar to one used in Karkoschka 2009 [12] (Figure 3) fits our data better than the profile from Irwin 2012 [14]. The corresponding model and the observed spectrum is shown in Figure 4.

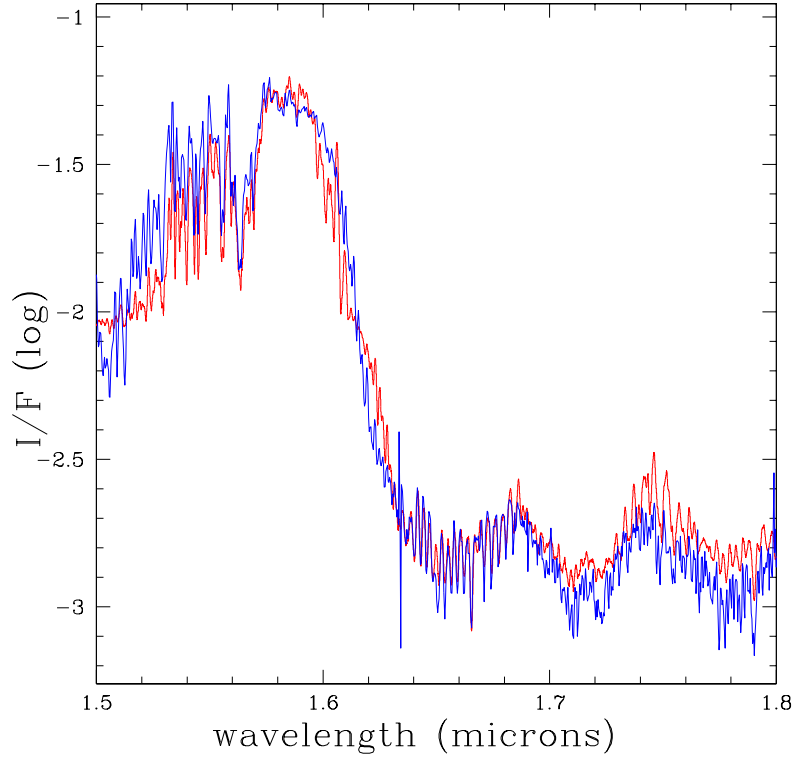


Fig. 4: A fit of the near-IR spectrum of Uranus (blue) with VSTAR (red). The updated methane profile gives better line amplitudes throughout and a much better fit around 1.65 microns.

Deuterium Abundances

The H-band region of the Uranus spectrum can be used to model the ratio of deuterium to hydrogen (D/H). This ratio is an important diagnostic, helping us to understand the process of Solar System formation. The D/H ratio combined with a solar nebula model provides insight into the formation of the giant planets, namely where they formed and through what means their deuterium is likely to have been trapped. [34] [35]

The new line data from Wang 2011 [29] provide identification of the $\text{CH}_3\text{D } 3\nu_2$ band in the $1.56 \mu\text{m}$ window. The most recent modelling of this band from the Gemini North NIFS data in Irwin 2012 [14] provided a D/H ratio in methane of 9.2×10^{-5} as compared with the D/H of the Vienna Standard Mean Ocean Water (V-SMOW) of 1.56×10^{-4} . Deuterium abundances decrease as we move away from the sun in the current Solar System formation model, therefore a vastly different D/H ratio could suggest that Uranus formed far from its current orbital distance. Uranus' spin-axial tilt, it has been suggested, could be due to collisions with large bodies [36], so it would not be entirely surprising if it did form at a different distance from where it currently sits and moved due to interactions with large bodies.

The preliminary model in Figure 4 was derived with a D/H of 7.5×10^{-5} notably further removed from the Earth abundance than the value of 9.2×10^{-5} from Irwin 2012 [14]. This was used because it provided us with an apparent best fit for the deuterium-sensitive H-band window, however this resolution of spectra is not sufficient to distinguish this value from previously estimated values. We are currently analysing high resolution data ($R \sim 18000$) of this region from Gemini North GNIRS from which we should be able to better confine the best fit for the D/H ratio. The model parameters from the IRIS2 data presented here will be used as starting parameters for the more detailed and refined model needed to fit the GNIRS spectrum. For icy objects this ratio is determined by the formation temperature and hence the orbital radius in the Solar System at which ice formed [37]. Hence, accurate measurements can provide information on the formation and early history of the ice giant planets, and in particular their possible orbital migration [22]. Our GNIRS data should enable improved determination of the D/H ratio due to its higher spectral resolution compared to the AAT IRIS2 data. The GNIRS observations were also obtained in good seeing conditions, and so have better spatial resolution, which will allow to apply more targeted model parameters for different ranges of latitudes.

Discussion and Conclusions

Our results show that a much improved model of the spectrum of Uranus in the H-band region can be achieved using the new methane spectral line data now available. Because this line data is not available at wavelengths shorter than $1.26 \mu\text{m}$, it is not currently possible to model the J-band data using these line-by-line techniques.

This type of model will be a valuable starting point for modelling the much higher resolution Gemini GNIRS data on Uranus that we have taken recently. These higher resolution spectra should enable much more accurate determinations of the D/H ratio and will also allow searching for other trace species that might be present in the atmosphere.

Uranus now joins a growing list of Solar System atmospheres that have been successfully

modelled with VSTAR and shows the versatility of the methods employed by the software. VSTAR allows the modelling of exoplanetary spectra, such as those that are now being obtained from transits and secondary eclipses. As has been shown in the modelling of the Solar System giant planets, the quality of the spectral line data is important in achieving successful results. While the methane line data are now good enough for accurate modelling of low temperature objects like Uranus, the line lists are still not sufficiently complete for high temperature objects such as hot Jupiters, where hot bands of methane become important. The design of VSTAR allows the easy inclusion of updated line lists as they become available, meaning that once these lists are developed, VSTAR will be ready to move on to exotic exoplanets.

We've produced a good fit to the observed spectrum with two cloud layers, the upper one of which being a thin haze-like layer, and an adopted mixing ratio. Further analysis is needed for the deuterium abundance to be well determined and any firm conclusions drawn about it. GNIRS observations already acquired will be analysed to pin down the deuterium abundance, although the IRIS2 data we've considered here has given us a firmer understanding of the structure and composition of the atmosphere, allowing us to more confidently fine tune the deuterium abundance. The implications of these findings however are of interest as the deuterium abundance can give us clues about where a planet has formed and under what conditions. [2] [14] [17] [22] [37]

Acknowledgments

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